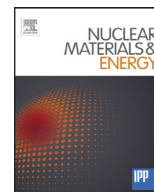




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Efficient code simulation strategies for B2-EIRENE

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ABSTRACT

Plasma edge simulation codes are crucial for the interpretation of present experiments as well as for the assessment of new concepts and next generation nuclear fusion devices. These codes are most often based on a combined Finite Volume (FV) / Monte Carlo (MC) numerical approach to simulate coupled plasma and neutral particle transport. In this paper we apply recently derived error reduction analysis to assess numerical errors in a partially detached ITER case. We show that also for this strongly coupled FV/MC simulation case, statistical averaging over iterations provides an accurate means to achieve well reproducible and statistically accurate results. Moreover, the error reduction analysis with respect to numerical parameters provide a framework to achieve increased accuracy for a given computational cost. We also show how significant code speed-up can be achieved for a desirable accuracy compared to presently used simulation strategies.

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1. Introduction

In fusion research, plasma edge simulation codes are used to evaluate vital aspects such as energy and particle exhaust, erosion of the plasma facing components, and the related migration and deposition of material. This is true for the analysis of present day experiments, for the evaluation of the operational window of the current ITER reactor, as well as for the design of the next generation reactor DEMO. To this end, B2-EIRENE [1] and its later versions SOLPS and SOLPS-ITER are, amongst others, used worldwide. However, both reliable error assessment and computational efficiency remain a challenging task. This is especially true in the case of strong coupling between plasma and neutral particle transport as present in the computationally demanding (partially) detached regime, the reference operational scenario for ITER and DEMO. Only recently, a systematic study on 1D test cases with a Finite Volume (FV) / Monte Carlo (MC) code system revealed theoretical error reduction rates induced by different coupling techniques (such as correlated sampling, random noise and Robbins Monro) [2,3]. The latter coupling procedure turned out to be slower than the first two coupling strategies. The correlated sampling coupling uses ensemble averaging of “frozen” noise simulations. However,

these “frozen” noise simulations are hard to achieve, especially when more atomic and molecular processes are added to the MC simulations. Moreover, it was shown that, for simple test cases, the random noise coupling procedure with averaging outperforms the correlated sampling coupling with respect to accuracy for a given computational cost. A simple 2D “slab” case studied with B2-EIRENE confirmed these findings [3]. A simple slab case was also studied in [4] to establish the effect of synthetic noise on statistically averaged solutions. These results constitute a promising starting point for a practical simulation procedure, in particular when using random noise coupling. However, their applicability to realistic plasma edge simulations remains to be demonstrated.

This paper fills this gap by assessing the use of a full random noise coupling procedure for a partially detached B2-EIRENE ITER simulation with respect to accuracy and computational cost. We show that, for this case, random noise coupling can result in more accurate simulations using a lower number of MC particle trajectories than traditionally used. The key is to not simply use the final result of the iterative procedure, but to perform an appropriate statistical averaging of the results over consecutive iterations. We show that such a procedure delivers well reproducible and statistically accurate results and paves the way for further code speed-up. Moreover, we illustrate that results from [3] provide a framework to assess the accuracy of such simulations in practical cases. This brings a positive perspective for further goal-oriented error reduction and code speed-up. In Section 2.1 we briefly summarize the

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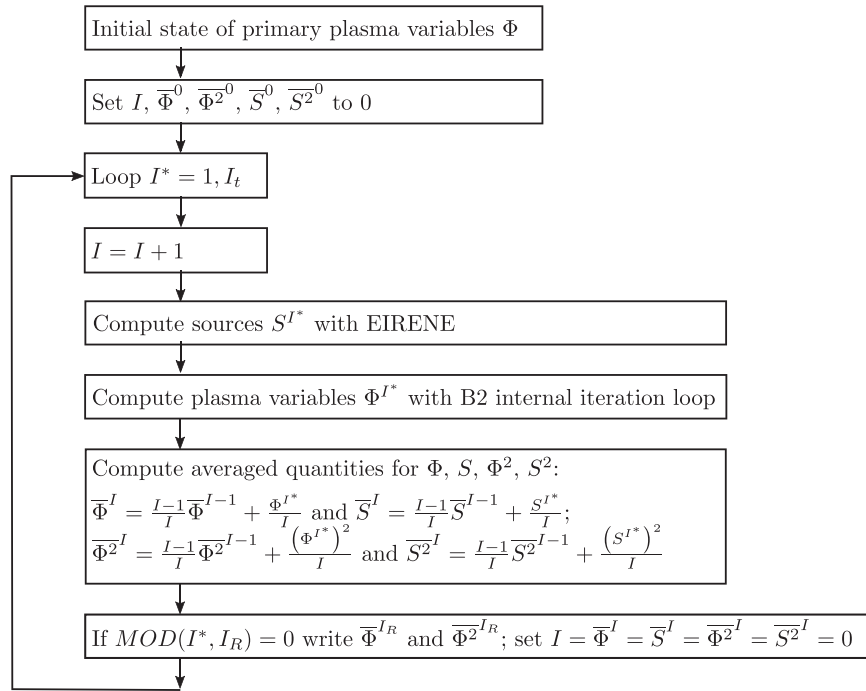


Fig. 1. Flow chart of the B2-EIRENE simulation run.

main features to set up a framework for error analysis related to the code coupling between FV and MC simulations. Next the ITER test case is described. In Section 3 the error reduction rates are investigated for this case. The involved errors for target plasma properties and integral target fluxes are assessed in Section 4. Finally, in Section 5, a simulation strategy is set up that allows starting from initially flat profiles, and achieves converged results in reduced computational time, while keeping the same accuracy as in the procedure used up to now.

2. Accuracy and code speed-up for coupled FV/MC ITER simulations

2.1. A framework for error analysis

In this paper we focus on the accuracy of the instantaneous solution Φ . This value Φ can be interpreted both as the outcome of the computation with respect to the primary variables such as local ion or neutral densities, velocity components or temperatures as well as any other quantity of interest such as heat load to targets, or pumped particle flux, etc. Following the conclusions from [2,3], we expect that on top of modelling errors (due to modelling inaccuracies) and discretization errors (due to finite grid resolution) a deterministic and a statistical error contribution on the FV/MC simulation results. These errors are caused by the noise introduced by the MC simulation technique. Averaging the instantaneous solution Φ , obtained on a specific grid with P tracked MC particles in every iteration, over I iterations leads to the averaged solution $\overline{\Phi}^I$ with reduced statistical error. In [2,3] it is found that both the deterministic and statistical error decrease according to specific trends. The deterministic error ϵ_{bc}^P is induced by two contributions: a lack of convergence and a finite number of MC particles. The first induces a so-called convergence error, while the latter induces a so-called finite sampling bias. This deterministic error is expected to decay inversely proportional to the increasing number of MC particles, i.e. $\epsilon_{bc}^P = \frac{A_{bc}}{P}$, with A_{bc} a constant value. The statistical error ϵ_s^P is associated with the statistical noise

introduced by the MC simulations to obtain the plasma particle, momentum and energy source terms from neutral-plasma interactions. This error is expected to vary with the number of MC particles P and the number of iterations I over which averaging is applied as

$$\epsilon_s^P \approx \sigma_{\Phi^I} = \frac{\sigma_{\Phi}}{\sqrt{I/\mathcal{T}}} = \frac{A_s}{\sqrt{PI/\mathcal{T}}}. \quad (1)$$

Here, A_s is a constant value, and \mathcal{T} is a factor to account for the fact that the instantaneous solution Φ is not independent from its previous values over subsequent iterations. This factor is related to the integral time scale T_I and the autocorrelation function $\rho(\tau)$ of the variable Φ [5]. However, evaluating the integral time scale via the autocorrelation, as proposed in [3], is a tedious procedure as all variable samples obtained through the iteration should be stored. This is in contrast to the averaged values and related variances that can be computed as the simulation proceeds. Indeed, the averaging procedure is an interpretative post-processing procedure, that does not interfere with the actual iteration procedure. It is depicted in the flow chart in Fig. 1. The averaging of all plasma variables takes place within each iteration and is stored as a separate quantity. The averaged value $\overline{\Phi}^I$ at iteration I^* can be obtained from the averaged value $\overline{\Phi}^{I-1}$ at iteration $I^* - 1$ and the instantaneous value Φ^{I^*} by $\overline{\Phi}^I = \frac{I-1}{I}\overline{\Phi}^{I-1} + \frac{\Phi^{I^*}}{I}$, with I the number of iterations over which averaging took place. This should clearly be distinguished from the overall number of iterations I^* already performed, as the averaging starts after a transient phase of I_{tr} only, i.e. $I = I^* - I_{tr} + 1$. This starting point for averaging I_{tr} is at present determined by monitoring several variables over the grid (i.e. at separatrix, outer mid-plane, corner cells, etc.). When these values demonstrate a statistical steadiness, the averaging of the plasma variables is started. It is clear that, in principle, only the mean value needs to be additionally stored for each variable during the run. However, in order to achieve a more practical procedure, we make use of batch means [6]: the iterations are divided in batches of I_R iterations and averaged quantities are computed for each batch. The overall mean value is subsequently computed as the average of these

batch means. The use of batches both facilitates the detection of the transient phase and the computation of the statistical error, as will be explained next.

Similar to the computation of the averaged values the variance, needed to assess the statistical error, is computed from the average of Φ^2 , i.e. $\overline{\Phi^2}$, by

$$\sigma_\Phi \approx s_\Phi = \sqrt{\frac{1}{I} \sum_{i=1}^I (\Phi - \overline{\Phi})^2} = \sqrt{\overline{\Phi^2} - \overline{\Phi}^2}. \quad (2)$$

The variance σ_Φ will depend on the numerical parameters used. In order to estimate the statistical error of the mean from this variance value, we exploit the variance obtained from the batch means too. When I_R is chosen sufficiently large to obtain independent batch means and sufficiently small to retain a sufficient number of batch means, $\sigma_{\Phi^{I_R}} = \sigma_\Phi / \sqrt{I_R/T}$. Thus, \mathcal{T} is approximated by

$$\mathcal{T} \approx \left(\frac{s_{\Phi^{I_R}}}{s_\Phi} \right)^2 I_R. \quad (3)$$

Here $\overline{\Phi^{I_R}}$ is the averaged value for each consecutive batch with I_R iterations. The statistical error on the mean value can then be assessed using Eq. (1). It should be stressed that this averaging procedure does not change the plasma state results Φ during the iterations. Instead, it provides the averaging information $\overline{\Phi^{I_R}}$ and $\overline{\Phi^2}^{I_R}$ that is needed for post-processing only.

2.2. Partially detached ITER test case

In the next section, we will demonstrate the applicability of error reduction analysis and its related accuracy assessment and code speed-up for a pure Deuterium plasma simulation under partially detached conditions on the ITER F12 geometry (# 2011) [7]. The geometry, shown in Fig. 2, is run with the SOLPS4.3 version of the B2-EIRENE code on a 74×28 grid. The starting point of our present study is the original simulation with a prescribed core ion particle flow $\Gamma_c^i = 9.1 \times 10^{21}$ #/s and ion and electron heat transfer rates from the core $Q_c^i = Q_c^e = 19$ MW each. The original results were obtained using dual time stepping (with 15 inner iterations), a time step for both inner and outer iterations of $\Delta t = 9 \times 10^{-7}$ s and a relaxation factor of 0.5. The EIRENE code is called every outer iteration. 70,000 particles are launched in every EIRENE call, based on a random seed initialization. It should be noted that typically the result of the last iteration is taken to be representative for the steady state solution. This simulation result is taken as the starting point for one series of simulations with averaging as described below.

Simulation results are shown with the same boundary conditions and numerical parameters, except for the number of particles launched in each EIRENE run. The number of particles is systematically decreased with a factor 10 from 70,000 particles down to a number as low as 70 launched particles. The latter is done in order to provoke the deterministic error in an extreme way. For this run the EIRENE run is accomplished so quickly that the use of the clock time to randomize the seed is not sufficient anymore. Indeed, it is observed that in this run with an extremely low number of MC particles, anomalies (such as sudden drops and peaks) are retrieved in the plasma profiles. These anomalies are caused by the correlation in subsequent seeds that now impact too much on the plasma solution obtained with iterative false time stepping. When the seed initiation number is increased every call with one unit, this correlation is avoided and the anomalies disappear. Two series of simulations are performed: one starting from the reference solution and one starting from flat initial plasma parameter profiles. The most accurate solution is obtained by continuing the

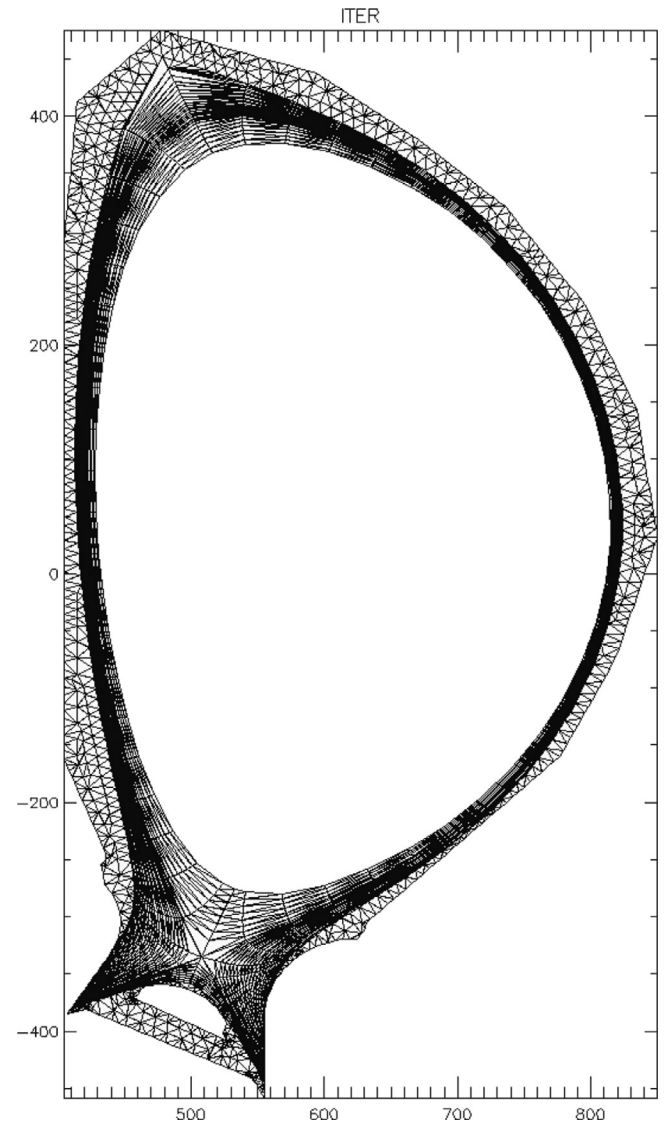


Fig. 2. R–Z poloidal plane of the simulated ITER geometry. The quadrilateral mesh is used for plasma simulations with the B2 code, while the grid is extended with a triangular mesh region for neutral particle transport computations with the EIRENE code.

original ITER simulation with 70,000 MC particles while averaging over 75,000 iterations. The averaged result will be taken as a reference to assess the errors for the different simulations.

Averaging is performed in a post-processing way. For $P < 70,000$, it is started after a transient phase of $I_{tr} = 150,000$ iterations. In order to assess the factor \mathcal{T} , batch means are evaluated every $I_R = 500$ iterations. The final averaged simulation result is taken as the overall average over the successive batch runs after $I_{tr} = 150,000$ iterations. This means that averaging is performed over $I = 350,000$ iterations, requiring in total $I_t = 500,000$ iterations.

3. Results

3.1. Rate of error reduction

The theoretical rates of error reduction with respect to the number of MC particles P and to the number of iterations I are now examined for the set of simulation runs started from the reference solution. To this end, the residual for the continuity equation is plotted in Fig. 3. The residuals are calculated from the

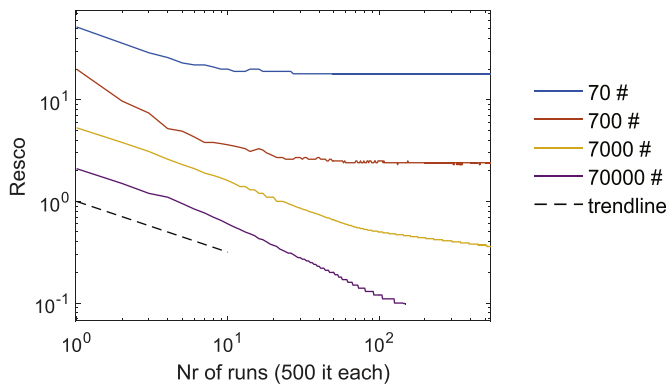


Fig. 3. Continuity equation residuals for averaged plasma variables $\bar{\Phi}$ and MC sources \bar{S} .

accumulated averaged plasma parameters $\bar{\Phi}$ (i.e. density, velocity and ion and electron temperatures) and the accumulated averaged plasma sources \bar{S} . These accumulated averaged values are computed using the batch averaged values. From the figure it can be seen that in the initial phase of the iterations the slope of the residuals is approximately governed by the $1/\sqrt{I}$ error reduction rate. Moreover, the lines for the different numbers of MC particles lie approximately a factor $\sqrt{P} = \sqrt{10}$ apart. At a higher number of iterations the residual stagnates. This is the phase where the deterministic error becomes dominant. It can be seen clearly that at these higher iteration numbers the residual (and with it the error) decreases inversely proportional with the number of MC particles: the lines now tend to be a factor 10 apart.

3.2. Simulation results

Simulation results for the different runs are summarized in Table 1. For all simulations the first column indicates the number of particles P and the total number of iterations I_t , except for the original ITER-simulation without averaging, which is indicated by $I_t = \text{ITER}$. Density, as well as electron and ion temperatures at the outer target at the separatrix strike point are listed in the second to the fourth column respectively. In the next columns total particle flux, as well as electron and ion energy fluxes to the outer target are given. In the last column a measure for the computational time is shown. This measure is expressed in overall number of MC particles (MCP) needed and is determined from $P(I_{tr} + I_{av})$.

From Table 1 it can be seen that the case with ($P = 70000$) achieves results with deviations from the reference solution of the same order of magnitude as for the original ITER case. The result can be obtained at a computational cost that is approximately 50% lower. This speed-up factor is not yet the maximum

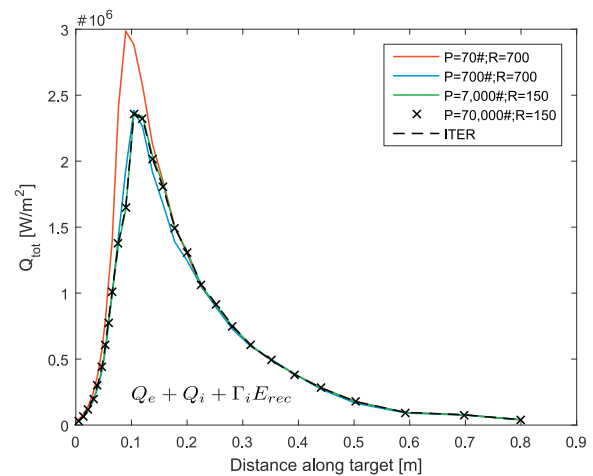


Fig. 4. Total heat flux density profile to the outer target.

code speed-up the error assessment can bring as the number of iterations executed for averaging in this example is taken arbitrarily at $I_{av} = 350,000$. Indeed, e.g. averaging over 75,000 iterations only yields similar simulation results at a computational cost that is now lowered by a factor 6. The error reduction rates will serve to further speed up the code by optimizing the setting for P and I_{av} , as will be explained in the next section. Furthermore, drastic code speed-up can be achieved, while keeping the deviations of the monitored plasma properties within 10%, by lowering the number of MC particles even more. Further, it is remarkable that similar results are achieved for both the ITER initial profile and the flat one: it is observed that the iterations needed for the transition phase are in the same order of magnitude for both simulations. Code speed-up amounts to a factor of 30 for $P = 700$. This means in practice, that this strongly coupled plasma-neutral particle simulation can be performed now from flat profiles in 100 hours for the $P = 700$ case on a DELL with Intel(R) XEON(R) CPU at 2.5 GHz using one processor only. Little can be gained in computational time by reducing the amount of particles further to $P = 70$. The computational time now equals 50 h only. This means that the MC runs are no longer dominating the overall computational cost.

The overall plasma heat profiles to the outer target and the associated electron temperature are shown in Figs. 4 and 5 for the first series. The overall plasma heat flux is defined as the sum of ion and electron heat fluxes to the target complemented with the energy loaded to the target from the ion particle flux recombining at the target (13.6 eV for the recombination energy per ion). For the overall heat flux all solutions agree well with the one from the original ITER simulation, except for the $P = 70$ case. The electron temperature loses accuracy for the $P = 70$ and $P = 700$ case

Table 1

Simulation results for different initial profiles and number of MC particles; $I_{tr} = 150,000$ for $P < 70,000$; $I_t = \text{ITER}$ refers to the original ITER-simulation without averaging.

Case ($P; I_t$)	$n_{i,sep}^{OT}$ $10^{20} \frac{\#}{m^3}$	$T_{e,sep}^{OT}$ eV	$T_{i,sep}^{OT}$ eV	Γ_{n_i} $10^{24} \frac{\#}{s}$	Q_e^{OT} MW	Q_i^{OT} MW	CPU MCP
Reference case (70,000; 225,000)	8.52	0.61	1.09	2.09	6.55	4.84	1.58×10^{10}
ITER profile (70,000; ITER)	8.52	0.61	1.08	2.09	6.57	4.85	1.1×10^{10}
(7000; 500,000)	8.40	0.61	1.08	2.07	6.60	4.83	3.5×10^9
(700; 500,000)	7.76	0.67	1.20	2.15	6.13	4.82	3.5×10^8
(70; 500,000)	7.83	0.99	1.77	2.21	7.55	5.44	3.5×10^7
Flat profile (700; 500,000)	7.84	0.65	1.16	2.09	6.28	4.80	3.5×10^8
(70; 500,000)	7.87	0.93	1.75	2.22	7.46	5.43	3.5×10^7

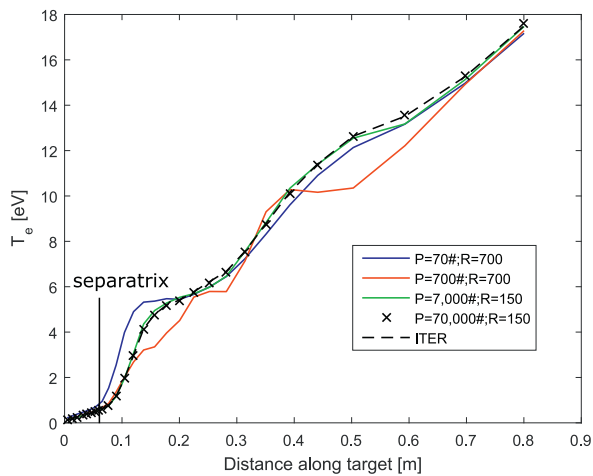


Fig. 5. Electron temperature along the outer target.

Table 2

Absolute relative errors as obtained from simulation results ($l_t = l_{tr} + l_{av}$; $l_{tr} = 150,000$; l_t = ITER refers to the original ITER-simulation without averaging).

Case (P ; l_t)	$n_{i,sep}^{OT}$	$T_{e,sep}^{OT}$	$T_{i,sep}^{OT}$	Γ_{n_i}	Q_e^{OT}	Q_i^{OT}
ITER profile						
(70,000; ITER)	0.01%	0.7%	0.7%	0.1%	0.3%	0.1%
(7000; 500,000)	1.4%	0.2%	0.4%	1.0%	0.8%	0.2%
(700; 500,000)	9.0%	9.7%	10.4%	3.0%	6.4%	0.5%
(70; 500,000)	8.1%	62.2%	63.1%	5.7%	15.3%	12.3%
Flat profile						
(700; 500,000)	8.0%	5.9%	6.6%	0.1%	4.1%	0.9%
(70; 500,000)	7.6%	52.3%	60.9%	6.0%	14.0%	12.0%

due to the higher fluctuations induced by the transitioning between attached and detached situation at positions outside from the separatrix strike point. This provides both larger deterministic and statistic errors in this region. However, the trend of partially detached divertor regime is kept in all cases.

4. Error assessment

In Table 2 the relative error $\delta = |\epsilon|/\Phi_{ref}$ is listed, with the absolute error $\epsilon = \Phi - \Phi_{ref}$, and Φ_{ref} the value of the reference solution. Especially for the most accurate simulations (cases (70,000; ITER) and (7,000; 500,000)) the difference is largely influenced by the error on the reference solution itself. Therefore these relative errors should be interpreted with caution. From the table it is clear that the simulations initiated with flat profiles perform equally well as the ones started from the original ITER solution. This confirms the conclusion of the previous section that fast exploration of ITER configurations, even in the partially detached regime, is enabled at a low computational cost by appropriate averaging.

Following the theory explained in Section 2.1, the constant values for the deterministic error are obtained from the theoretical error reduction expressions, by taking the difference of the result obtained with $P = 700$ with the reference case. The constant value for the statistical error is computed via Eqs. (3) and (1), using again the $P = 700$ case. The obtained numerical constants are listed in Table 3 for the plasma variables at the outer target separatrix position and the integrated fluxes along the target. As the variance was only monitored for primary plasma variables, \mathcal{T} cannot be evaluated. Therefore it is taken as a rough estimate from the primary variables. The resulting theoretical relative errors are displayed in Table 4. The predicted errors are of the same order of magnitude as the observed ones, except for some of the $P = 70$ simulations, where the observed errors are smaller than the expected ones. This

Table 3

Numerical constants for error assessment.

	$n_{i,sep}^{OT}$ $10^{20} \frac{\#}{m^3}$	$T_{e,sep}^{OT}$ eV	$T_{i,sep}^{OT}$ eV	Γ_{n_i} $10^{24} \frac{\#}{s}$	Q_e^{OT} MW	Q_i^{OT} MW
A_s	16	1.6	2.9	0.6	4.7	1.2
A_b	560	42	70	43	291	18
\mathcal{T}	14	27	37	≈ 20	≈ 20	≈ 20

Table 4

Relative errors as predicted by theory; l_t = ITER refers to the original ITER-simulation without averaging.

Case (P ; l_t)	$n_{i,sep}^{OT}$	$T_{e,sep}^{OT}$	$T_{i,sep}^{OT}$	Γ_{n_i}	Q_e^{OT}	Q_i^{OT}
(70,000; ITER)	0.8%	1.1%	1.1%	0.1%	0.3%	0.1%
(7000; 500,000)	1.0%	1.0%	1.0%	0.3%	0.6%	0.1%
(700; 500,000)	9.4%	9.8%	9.3%	3.0%	6.4%	0.5%
(70; 500,000)	94.0%	98.0%	92.3%	29.4%	63.5%	5.3%

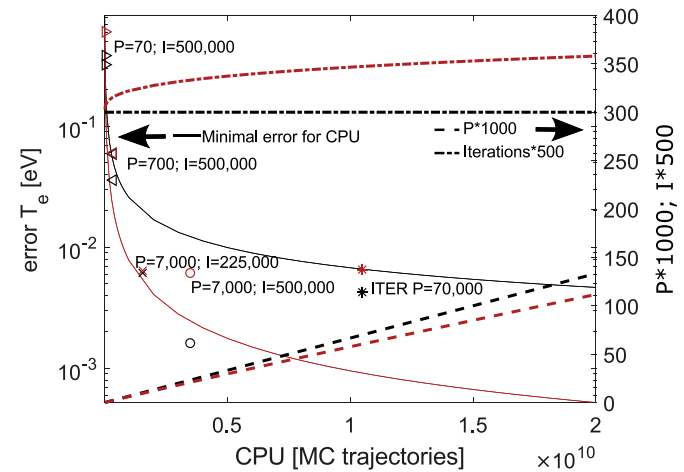


Fig. 6. Accuracy ϵ_t (solid line), total number of iterations $I - t$ (dash-dotted line) and number of particles P (dashed line) versus computational cost for standard use of B2-EIRENE (black) and under optimal averaging parameters (red); markers indicate position of present simulations as observed (black) and as predicted by theory (red). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

is related to the observation that the theoretical error reduction scaling for this small number do not hold anymore, and is most probably caused by second order effects as the plasma variables strongly fluctuate over the iterations.

5. Optimal strategies

From the previous results it becomes apparent that the computational cost required for a coupled FV/MC simulation as provided by B2-EIRENE is largely depending on the required accuracy. The theoretical error reduction scaling now provide a tool to optimize the numerical parameters of the averaging procedure, i.e. P and l_{av} . Indeed, as the total error of the averaged value of interest can be expressed by $\epsilon = \frac{A_s}{\sqrt{Pl_{av}/\mathcal{T}}} + \frac{A_{bc}}{P}$, while the computational cost is governed by $P(l_{tr} + l_{av})$, an optimal $P - l_{av}$ combination can be found for a desired accuracy. The optimal line is plotted in Fig. 6 for the electron temperature at the outer target separatrix strike point, given the transient phase in the simulations of $l_{tr} = 150,000$ iterations. It should be noted that for other physical quantities of interest different results might be obtained as the error is strongly related to the variance of the quantity. On the same graph the accuracy as obtained by the original procedure $\epsilon = \frac{A_s}{\sqrt{P}} + \frac{A_{bc}}{P}$ is shown. Furthermore, the dashed lines show the number of particles to be used, while the dash-dotted lines

represent the total number of iterations I_t needed. Depending on the required accuracy the computation can be speeded up under optimal conditions by an order of magnitude or for the same computational cost the accuracy can be increased by one order of magnitude. These non-optimized simulations as presented in this paper are also shown on the graph (with black markers), together with the theoretical error and CPU value (with red markers). As already explained in Section 4, it is noted that the calculated relative error for the $P = 70,000$ and $P = 7,000$ simulations (black markers) suffer from inaccuracy of the reference solution and may therefore deviate from the exact ones. For the ITER run it is assumed that the simulation is taken immediately after the transient phase. This was most probably not the case in this ITER simulation, as the monitoring tool was not available. As such it provides a lower limit for the CPU spent in the past. Finally, from the graph it becomes clear that the high P simulations can be further speeded up without loss of accuracy, as they have been too long averaged over iterations. All these considerations can lead to a code speed-up higher than the ones reported in Section 3.2.

6. Conclusions

In this paper we show how theoretical error reduction scalings can serve to determine the errors of simulated quantities with a FV/MC coupled edge plasma code induced by a finite number of MC particles. The procedure is demonstrated for an ITER simulation with B2-EIRENE. Low MC particle runs are used to assess the deterministic error associated with finite sampling and convergence during the random noise coupling procedure. It is concluded that post-processing averaging over iterations is key to increase accuracy or to speed up the simulations. The averaging procedure shows to provide reliable results, even for the partially detached outer divertor regime as used in this test case. Finally, it is shown how an optimal simulation strategy can be followed for any parameter of interest.

The optimal strategy might be further extended to a multi-step approach. Moreover, given the short simulation times, grid sensitivity studies come within reach. Both topics will be subject for further research. In a next step, this averaging procedure will be made available in the SOLPS-ITER code.

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